

Location of Copper Cations in Synthetic Faujasite Zeolite-X Using XAS	X18B
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The sodium in zeolite-X was fully exchanged with copper. The samples were calcined then eluted with ammonium chloride to remove copper from open sites (super-cages) of the zeolite. The remaining copper cations were in locked sites (sodalite-cages or hexagonal-prisms). Using XAS edge-jump we found that 22.0, 23.5, 24.5, 24.6 and 28.3 copper cations were locked at 43, 73, 112, 150 and 195 deg C respectively. The analysis of the first shell Fourier Transformed radial distribution show that cations at site I in the hexagonal-prism and site II in the sodalite-cages, adjacent to site I, are distributed at equal proportion, independent of temperature. Considering the fully exchanged copper zeolite as 100% the locked site of the calcined samples at 43, 73, 112, 150 and 195 deg C were 63, 67, 70, 71 and 81 percent respectively. The Fourier Transform of these spectra show an average height of the first peak equal to 0.1378 with the mean standard deviation of .0019 (1.4% within this deviation, the copper cations are distributed at an equal proportion between the site I and site II. The cations which occupy the hexagonal prisms are expected to have twice the coordination number as compared to the site II in the sodalite cage. An uneven cation distribution will give rise to different peak heights. Assuming that the maximum number of copper cations that can be exchanged in zeolite X is 35 (Lai et al, J. Chem. Soc. Faraday Trans. 72, 1809-1817, 1976), the number of copper cations locked corresponding to these percentage is 22.0, 23.5, 24.5, 24.6 and 28.3 for the above calcined temperatures respectively. However, there is a great discrepancy between the results reported here and the one reported by the above authors. We find our results much higher than what Lai et al reported from their experiments. One possible reason could be that the hydrogen ion from water at different treatment levels was occupying the positive cation sites of the zeolites and in that process was giving rise to a higher percentage of occupied sites. The important observation from our experiment was the consistent increase in the edge-jump of the copper spectra with the increase in temperature and the constant height of the first shell of the radial distribution within 1.4% discrepancy between our results and the one reported by Lai et al. We will also use this technique to find the distribution of other cations in this and other zeolites.